

## LA-UR-19-22172

Approved for public release; distribution is unlimited.

Title: FEARCE Development - Institutional Computing Report for 2019

Author(s): Carrington, David Bradley

Intended for: Report

Issued: 2019-03-12

---

**Disclaimer:**

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

## FEARCE Development - Institutional Computing Report for 2019

PI: David B. Carrington

T-3 Fluid Dynamics and Solid Mechanics

**FEARCE** (Fast, Easy, Accurate and Robust Continuum Engineering) software is designed to solve turbulent reactive flow with a particular emphasis on flow with aerosols, sprays, injection, and moving mechanical components, which are internal combustion engines, like those in our cars and trucks. FEARCE can be used to optimize the design of internal combustion engines, looking to increase efficiency and reduce emissions.

The software uses a finite element method which allows many advantages over other simulation or modeling techniques, particularly in the following ways: 1) the scalability of the software on parallel machines, 2) the ease of performing higher accuracy simulations, and 3) ease of creating simulated parts or engines; the grid generation. A rather unique method to the engine modeling community is how FEARCE handles moving parts in a robust and accurate manner, never failing during simulation (robust). The unique immersed moving parts methods facilitates the ease of grid generation. FEARCE includes high fidelity chemical reaction kinetics to enable evaluation of emissions providing for development of cleaner, more efficient engine design and the use of new fuels, such as biofuels or even multiple fuels at once.

The Department of Energy's Vehicle Technology Office sponsoring the FEARCE development works toward improving the efficiency of internal combustion engines as being one of the most promising and cost-effective near- to mid-term approaches to increasing highway vehicles' fuel economy. The Vehicle Technologies Office's research and development activities that includes FEARCE support addresses critical barriers to commercializing higher efficiency, very low emissions advanced internal combustion engines for passenger and commercial vehicles. FEARCE has received on average about \$650,000.00 per year over the last 9 years, or about \$5,850,000.00 dollars for development from DOE as the sole source of funding.

FEARCE simulates turbulent reactive flow, such as fluid dynamics and reactions that occur in internal combustion engines. We call this type of flow turbulent, reactive having multiple species (air, gasoline, carbon dioxide, water and hundreds of others), multiphase (liquid and gas) fluid flow. In particular it is flow related to engines with an emphasis on internal combustion engines, for example, gasoline and diesel engines found in cars and trucks. But the applications are not limited to these engines, large bore engines found in ships or trains can also be simulated as could turbines, gas burners, heaters, boilers, etc...

FEARCE uses a unique Vreman dynamic LES method allowing for modeling of unsteady flow, and flows varying from laminar to high turbulent; allows for highly varying flow modeling. Also included as options for less resolved engineering solutions are RANS models of  $k-\omega$  and Shear Stress Transport (SST)  $k-\omega$ .



Figure 1. Turbulence and mixing (vorticity) in a 4-valve direct injected spark ignited General Motors gasoline engine

In FEARCE there are 3 methods that maybe used to model the spray injection process. Two are engineering models, one called a Taylor-Analogy (TAB) and the other a Kelvin Helmholtz- Rayleigh Taylor model (KH-RT). These models use a stochastic Lagrangian Particle System that tracts, diffuses and also applies turbulent dispersion to parcels representing many particles with properties distributed about a mean. The droplets affect the motion of the fluid as they pass through, and the fluid of course affects the fluids motion. A two-coupling between the droplets and fluid media is created by balancing the forces on each. Unique to FEARCE's FEM system, the fluid and droplet properties are evaluated at the location they reside, the fluid is treated as a continuum, continuously varying within each small element representing the fluid in that portion of the problem. This is quite different than other methods that rely on nearest node or element property, as other methods are not truly representing the fluid as continuous, merely piecewise or element wise averages. This allows for more accurate particle transport and fluid-droplet force balances.

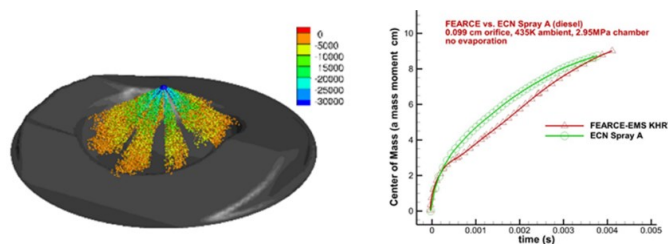


Figure 2. KH-RT injected liquid jet break-up and spray atomization in FEARCE

The other or third method for modeling the spray injection process, the break-up of the liquid jet to large drops can also be performed with an accurate Volume-Of-Fluids (VOF) method, calculating the exact forces on the liquid jet and large drops to break them into smaller droplets. VOF results match DNS on a relatively coarsely resolved domain.

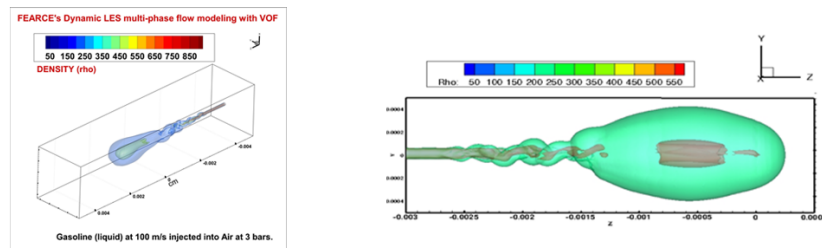


Figure 3. Liquid jet break-up in gas using FEARE's VOF, centerline slice of a 3D solution showing very high density

## FEARCE Development - Institutional Computing Report for 2019

A droplet vaporization modeling process is borrowed from KIVA-4 which evaporates fuel burn is simulated with a chemical kinetics portion of the software or other add-on software. Burning the simulated evaporated gases supplies heat, creating pressure onto the piston from which work is extracted. These thermodynamic and fluid dynamic processes are accurately modeled, including the turbulence of the fluid and fuel mixtures as they move through the engine system.

Pistons compress the fluid to high pressures and temperature before ignition of the fuel starts. Valves open and close controlling the inflow and outflow of the fluids while also promoting mixing. Pistons also extract energy released from the burning fuel as higher pressure drives the piston downward, expanding the volume and converting the energy released into work. These processes are modeled or simulated in FEARCE with a sophisticated calculus, called an immersed boundary method. There are 2 options for this in FEARCE, one using interpolating polynomials to evaluate the current state of the fluid in the neighborhood of the moving parts, and the other use special polynomials and a fictitious force method, called an immersed boundary FEM method. The latter method is the most accurate, but come with some extra cost of evaluating the entire domain as opposed to just those fluid elements that currently are part of the engine processes (those above the piston or active cells). This system is unique to FEARCE and the engine modeling community, where the standard for years has been the ALE method and recently the cut-cell systems.

FEARCE investigates turbulent flows in fuel combustion, such as fuel injection and fuel-air mixing, thermodynamic combustion losses, and combustion-emission formation processes in engines. We aim to understand turbulent flows and how they react and interact with other complicating variables, including highly nonlinear heat and mass transfer, small-scale velocity, and chemical kinetics or reactions.

Our novel computational fluid dynamics software models an engine's operating properties and ranges that can't be addressed with experiments. These simulation tools allow us to benchmark areas of most interest for engine operation before experiments are conducted. We also use these software tools to understand or analyze experimental data from our collaborators.

Engine designers use the simulations to optimize engines for increased fuel efficiency and reduced emissions, to understand how changes affect the efficiency and operation of engine. Use of FEARCE enables the designers to develop engines using other fuels, such as biofuels. Improving the efficiency of internal combustion engines is one of the most promising and cost-effective near- to mid-term approaches to increasing highway vehicles' fuel economy. The DOE's Vehicle Technologies Office's research and development activities address critical barriers to commercializing higher efficiency, very low emissions advanced internal combustion engines for passenger and commercial vehicles.

To run efficiently on computers, millions of cells require many processing elements or computational units, CPU's or computational nodes. The large domain is split up onto these CPU's for solution, 1000's of elements going to each CPU or computer node where the solution is solved. Each CPU's solution is communicated to the other CPU's for aggregation of the whole, done by a Message Passing Interface or MPI. The unique way FEARCE does this process made possible by the choice of solution methods, FEM, makes that domain splitting very efficient, better than the doubling idea where a double in problem size and number of processors for a given problem doubles the time it takes to solve, called a naïve or weak scaling. In fact, FEARCE is superlinear, falling well below this linear curve, and has almost a flat response when using sophisticated equation solution systems like multi-grid methods. This is just one example of the wins FEARCE has over its competitors, for which none generally develop a superlinear behavior.

The representation of the physics, the domain and the moving parts on the computer is binary, but the software is written in a computer language (FORTRAN 95) that a compiler interprets and converts to binary instruction sets, or machine language. FEARCE is written in this Fortran language in a modular way, with the FEM workings deep within the code, where people don't have to work, it is the machinery of the approximation not requiring adjustment as models are changed or added at the higher level of the code. The code is therefore consider to be leveled and modular, both desirable features of a modern day software.

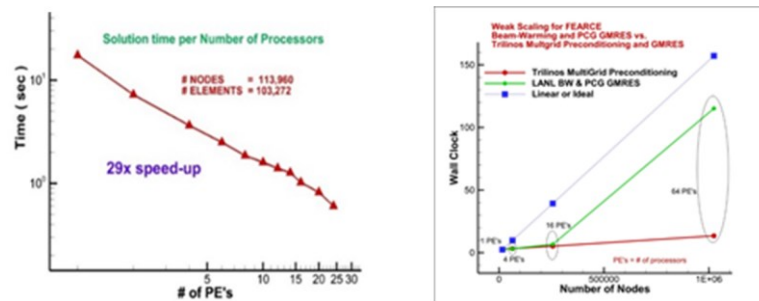


Figure 4. FEARCE scaling a) strong (same size more processors) showing super linearity of algorithm b) weak (size and processors doubling) showing superlinear algorithm and no preconditioning and very flat response to double with multigrid preconditioning

FEARCE allows for both AMR (h-adaptive) and Higher Order (HO) approximation (p-adaptive). FEARCE employs an not only an automatic grid refinement process (increasing or decreasing the resolution) based on error analysis as mentioned previously but, can increase the order of approximation. That is increase or decrease the order of the polynomial being used to approximate the variables be solved as the solution is running. Changing the approximation is performed with an error analysis also previous mentioned. FEARCE can use a combine h and p for hp-adaptive FEM. The real benefit comes with the combination of h and p adaptation. The grid refinement only produces a 2<sup>nd</sup> order convergence, but has low computational cost. This accuracy is shared amongst the competitors. However, adding HO approximation produces exponential convergence to the order of the approximation but by itself HO is pretty expensive in computational cost and speed of solution. Combining h-adaptive and p-adaptive methods provides for exponential convergence, grid resolution where required and much less computational cost, in other word as shown in the chart, hp-adaptive is on the same convergence cure as p-adaptive with less computational cost and time spent in the solution process

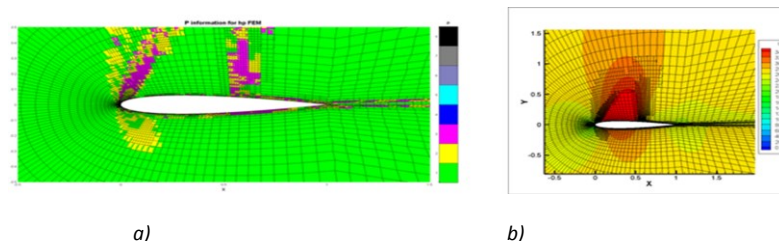


Figure 5. FEARCE's hp-adaptive system at work resolving the shocks created by near sonic flow over an wing a) up to 8<sup>th</sup> order approximation (black color at the leading edge) and the grid resolution around the shocks b) axial velocity isotachs showing the supersonic region between the shock regions.

## FEARCE Development - Institutional Computing Report for 2019

1. Wang, X., Carrington, D.B., Pepper, D.W., "Modeling Turbulent Compressible Flow with Thermal Effects using an hp-Finite Element Technique," International Journal of Computational Thermal Sciences, Begell House Inc., paper # CTS-28935, to appear.
2. Carrington, D.B., Waters, J., "Turbulent Reactive Flow Modeling in Engines: a robust and accurate Toolkit/software for simulating engine dynamics," *Proceedings of the ASME 2018 Internal Combustion Fall Technical Conference, ICEF2018*, November 4-7, 2018, San Diego, CA, USA, 2018
3. Hatamipour, V.D., Carrington, D.B., Heinrich, J.C., "Accuracy and Convergence of Arbitrary Lagrangian-Eulerian Finite Element Simulations based on a Fixed Mesh," Progress in Computational Fluid Dynamics, an Int. Jour., vol. 18, no 4, pp. 215-231, 2018
4. Carrington, D.B., Mazumder, M., Heinrich, J.C., "Three-Dimensional Local ALE-FEM Method for Fluid Flow in Domains Containing Moving Boundaries/Objects Interfaces," Progress in Computational Fluid Dynamics, an Int. Jour., vol. 18, no 4, pp. 199-215, 2018
5. Waters, J., Carrington, D.B., Wang, X., Pepper, D.W., "A Dynamic LES Model for Turbulent Reactive Flow with Parallel Adaptive Finite Elements," **Energy for Propulsion, Chapter 3: Turbulent Combustion Modeling and Simulations**, Springer, Singapore, pp. 217-235, 2018
6. Waters, J., Carrington, D.B., "Modeling Multi-Phase Flow: Spray Break-up Using Volume of Fluids in a dynamic LES FEM method," *2018 AIAA Aerospace Sciences Meeting, AIAA Science and Technology Forum and Exposition 2018*, Kissimmee, Florida, January 8-12, 2018
7. Waters, J., Carrington, D.B., Francois, M.M., "Modeling Multi-phase Flow: Spray Break-up Using Volume of Fluids in a Dynamic LES FEM method," Numerical Heat Transfer, Part B, vol. 72, no. 4, pp. 285-299, 2017
8. Waters, J., Carrington, D.B., "A Dynamic Large Eddy Model for Simulating Turbulent Reactive, Flow in Engines: A Parallel adaptive Finite Element Method," *Proceedings of WCX™17: SAE International World Congress Experience*, April 2-4, 2017 Detroit, MI, USA
9. Waters, J., Carrington, D.B., Wang, X., Pepper, D.W., "A Dynamic Large Eddy Model for Simulating Turbulent Reactive Flow with an Adaptive Finite Element Method," *Proceeding of the 2<sup>nd</sup> Thermal and Fluid Engineering Conference, TFEC2017*, April 2-5, 2017, ASTFE, Las Vegas, NV, USA
10. Waters J., Carrington, D.B., Pepper, D.W., "An Adaptive Finite Element Method with Dynamic LES for Incompressible and Compressible Flows," Journal of Computational Thermal Sciences, Begell House Inc., Vol.8(1), pp.57-71, 2016
11. Waters J., Carrington, D.B., "A parallel Large Eddy Simulation in a finite element projection method for all flow regimes," Numerical Heat Transfer, Part A, vol. 70, n0. 2, pp. 117-131, 2016
12. Waters, J., Carrington, D.B., "Modeling Turbulent Reactive Flow in Internal Combustion Engines with an LES in a semi-implicit/explicit Finite Element Projection Method," *Proceedings of the ASME 2016 Internal Combustion Fall Technical Conference, ICEF2016*, Oct 9-12, Greenville, SC, USA, 2016
13. Waters J., Carrington, D.B., "Parallel Large Eddy Simulation for Modeling 3D Turbulent Flow in Engines," *Proceedings of the ASME 2016 Fluids Engineering Division Summer Meeting*, July 10-14, 2016, Washington, DC, 2016
14. Waters, J., Carrington, D.B., Pepper, D.W., "An Adaptive Finite Element Technique with Dynamic LES for Incompressible and Compressible Flows," *Proceedings of the 15th Computational Heat Transfer Conference, CHT-15*, Piscataway, New Jersey, May 25-29, 2015.
15. Waters J., Carrington, D.B., Pepper, D.W., "Application of a dynamic LES model with an H-adaptive FEM for fluid and thermal processes," *Procs. of 1st Thermal and Fluid Engineering Summer Conference - TFESC*, 2015-08-09/2015-08-12, N.Y., N. Y., United States, 2015
16. Waters J., Carrington, D.B., Pepper, D.W., "Parallel Large Eddy Simulation for Turbulent Reactive Flow Modeling," *Procs. of the Int. Conf. Computational & Experimental Engr. & Sci. (ICCES'15)*, Reno, NV., 2015
17. David Carrington, Xiuling Wang, Darrell Pepper, "An hp-adaptive Predictor-Corrector Split Projection Method for Turbulent Compressible Flow," *Proceedings of the 15th International Heat Transfer Conference, IHTC-15*, Kyoto, Japan, August 10-15, 2014.
18. David B. Carrington, Xiuling Wang, Darrell Pepper, "A predictor-corrector split projection method for turbulent reactive flow," Journal of Computational Thermal Sciences, Begell House Inc., vol 5, no. 4, pp.333-352, 2014
19. David B. Carrington, Dominic Munoz, Juan Heinrich, "A local ALE for flow calculations in physical domains containing moving interfaces," Progress in Computational Fluid Dynamics, an Int. Jour. vol 14, no, 3, pp. 139-150, 2014